The Principle of Pooled Calibrations and Outlier Retainment Elucidates Optimum Performance of Ion Chromatography

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A new principle of statistical data treatment is presented. Since the majority of scientists and costumers are interested in determination of the true amount of analyte in real samples, the focus of attention should be directed towards the concept of accuracy rather than precision. By exploiting the principle of pooled calibrations retaining all outliers it was possible to obtain full correspondence between uncertainty of calibration and uncertainty of repetition, which for the first time evidences statistical control in experiments of ion chromatography. Chloride, bromide and oxalate were determined at a high number of repetitions in standards containing different anions. The method was capable of baseline separation of 17 different anions. It was found that the limit of quantification (LOQ) was significantly underestimated by up to an order of magnitude with respect to determination of concentration of unknowns. The concept of lower-limit of analysis (LLA) and upper-limit of analysis (ULA) were found to provide more acceptable limits with respect to reliable analysis at a limited number of repetitions. These findings comply with earlier investigations of method validations where it was found that the principle of pooled calibrations provides a more realistic picture of the analytical performance with the drawback however, that generally higher levels of uncertainties should be accepted, as compared to contemporary literature values. The implications to the science of analytical chemistry in general and to method validations in particular are discussed.